

23<sup>th</sup> September 2016 - 10:30 h

CFEL – Building 99, seminar room IV (1<sup>st</sup> floor)

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### Orientation of gas-phase proteins in static electric field studied using molecular dynamics simulations

Gas-phase structural biology enables the study of macromolecular systems that are otherwise challenging or impossible to interrogate. Charged gas-phase molecules are routinely separated using electric fields. Macromolecules also often carry a dipole moment, which could be used to orient them. To date the effects of strong fields on macromolecular structure are largely unknown.

Our calculations demonstrate the impact of dipole orientation for ion mobility spectrometry. We also show that it provides several benefits to diffractive imaging with X-ray free-electron lasers.

Using molecular dynamics simulations, we monitor the orientation and stability of four proteins exposed to electric fields in vacuum. We find that lower field strengths are required to orient proteins than those leading to unfolding. These findings can instruct the development of methods and instruments for gas-phase separation and structural interrogation of macromolecules.

